

R-Process Freezeout, Nuclear Deformation, and the Rare-Earth Element Peak

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Abstract

We use network calculations of r-process nucleosynthesis to explore the origin of the peak in the solar r-process abundance distribution near nuclear mass number $A \approx 160$. The peak is due to a subtle interplay of nuclear deformation and beta decay, and forms not in the steady phase of the r-process, but only just prior to freezeout, as the free neutrons rapidly disappear. Its existence should therefore help constrain the conditions under which the r-process occurs and freezes out.

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The r-process is responsible for synthesizing roughly half the heavy nuclei in the solar system (see Refs. [1,2] for a review). It is widely believed to occur somewhere in core-collapse supernovae, at a time when the density of free neutrons is so high that neutron capture by nuclei occurs much more rapidly than nuclear β decay. Under these conditions equilibrium between neutron capture and photodisintegration (called $(n, \gamma) - (\gamma, n)$ equilibrium) establishes itself so that very neutron-rich isotopes of each element are populated. The nuclei eventually β^- decay, turning one of their neutrons into a proton, then resume capturing neutrons until equilibrium is reached again. This “steady” phase of the r-process continues as long as the free neutrons remain abundant. When the neutrons begin to disappear, $(n, \gamma) - (\gamma, n)$ equilibrium becomes more difficult to maintain and β decays play a larger role in determining the most abundant isotopes of a given element. Eventually the neutron-capture and photodisintegration reactions “freeze out”, and the nuclei simply β -decay back to the stability line.

Large peaks in the solar r-process abundance distribution at nuclear mass numbers $A \approx 80$, 130, and 195 are apparently due to closed neutron shells. Closed-shell nuclei made during the r-process have strongly bound neutrons and long β -decay lifetimes, causing their abundance to build up. The source of a smaller peak at $A \approx 160$, the region of rare-earth elements (REEs), is far less clear. The authors of Ref. [3] speculated the cause to be deformation of neutron-rich REE nuclei. Beyond the closed shell at neutron-number $N = 82$, in this scenario, the stabilizing effect of deformation allows many more neutrons to be captured. When A reaches about 160, however, the nuclei can deform no further, and so add neutrons with difficulty, often β -decaying instead. The nuclei populated just past the deformation maximum therefore ought to be closer to the valley of stability than their predecessors and consequently should have somewhat longer β -decay lifetimes, leading to a moderate build up as the r-process proceeds. The calculations of [4] lent this hypothesis some support, but produced a much broader abundance hump than was observed and was unable to reproduce other r-process features.

An alternative explanation, first proposed in Ref. [5] and elaborated in Ref. [6], is that the REE peak is produced by mass-asymmetric fission of very heavy r-process nuclei. The fission fragments form a double-peaked abundance distribution in nuclear mass number, and the heavier products are supposed to fill in the r-process abundance curve at the location of the REE peak. By now, however, this idea is not compelling. As neatly pointed out in Ref. [7], the r-process should terminate by β -delayed fission before $A \approx 160$ fission fragments can be produced, and the small odd-even effect in the $A \approx 150 - 170$ region would be erased by fission. The source of the REE peak has therefore never been satisfactorily explained.

Despite the lack of an explanation, recent r-process simulations [8,9] in the high-entropy neutrino-driven bubble near the surface of the remnant neutron star have produced a nice REE peak. The simulations used calculated nuclear properties (far from stability) in which the effects of deformation had been included self-consistently. Significantly, however, the simulations did not allow nuclear fission. Moreover, they were among the first to follow the r-process all the way through freezeout. All this suggests that nuclear deformation, not fission, is responsible for the REE peak, but that the dynamics leading to freezeout rather than the mechanism of Ref. [3] cause it to form. In this paper we confirm and explicate this idea.

Our conclusions are based on an analysis of the development of the r-process “path”,

which we define as follows: At any given time, for each element with proton number Z , there is an isotope with maximum abundance; the collection of all such isotopes defines the path at that time. Before freezeout, when β -decay rates are much less than neutron-capture or disintegration rates and the system is in $(n, \gamma) - (\gamma, n)$ equilibrium, the path's location follows from the requirement that the free energy be stationary under the transfer of a neutron from a nucleus to the free-neutron bath. In the approximation that the nuclei and free neutrons in the r-process are ideal gases this condition, which is equivalent to detailed balance, implies that for every Z the isotope with maximum abundance has a neutron separation energy given by

$$S_n(Z, N_{max}) = -kT \ln \left\{ \frac{\rho N_A Y_n}{2} \left(\frac{2\pi\hbar^2}{m_n kT} \right)^{3/2} \right\}, \quad (1)$$

where N_{max} is the neutron number of the isotope, T is the temperature, ρ is the mass density, N_A is Avagadro's number, Y_n is the abundance of free neutrons per nucleon, and m_n is the neutron's mass. Eq. (1) implies that in equilibrium the path always lies along a contour of constant separation energy.

The high-entropy r-process calculations of Refs. [8,9], which showed a REE peak, were performed within detailed simulations of supernova explosions. Here we simplify matters by ignoring supernova fluid dynamics, instead parameterizing the dependence of temperature on time (with $\rho \propto T^3$) to roughly match the results of the more complicated calculations. We then use a computer code developed at Clemson University to solve the differential equations (described in Ref. [1]) that determine the time-development of nucleosynthesis. The inputs, besides the temperature and density, are the initial mass fractions of neutrons and preexisting "seed" nuclei, and calculated neutron capture rates [1], neutron separation energies [10], and β -decay rates [10]. The seed nuclei quickly come into $(n, \gamma) - (\gamma, n)$ equilibrium and then undergo the usual β -decay and neutron-capture sequence. We run the simulations through freezeout until only stable nuclei remain. The treatment of freezeout is fully dynamical in that neutron capture and photodisintegration continue to compete with β decay throughout the entire process, even when equilibrium no longer obtains. In the more detailed supernova simulations, the high-entropy r-process occurs over several seconds, and many r-process components combine to give the final abundance distribution (see, e.g., figure 15 of Ref. [9]). The calculations presented here treat just the components with the highest initial neutron/seed nucleus ratios, because they are responsible for the REE peak.

A sample set of predicted r-process abundances appear in figure 1a alongside the measured solar-system abundances. In this run the initial seed nucleus was ^{70}Fe and the initial value of R , the ratio of the abundance of free nucleons to that of nuclei, was 57, implying that a seed captured on average 57 neutrons. The very poor agreement just above the peak at $N \approx 82$ ($A \approx 130$) is unexplained but apparently plagues all such simulations. It may be due to a deficiency in the nuclear mass extrapolation [11] or the neglect of a second component with slightly different temperature and neutron density. In any event, we wish to draw attention here to the presence of a REE peak at approximately the correct location and with the correct width. No sign of this peak exists during the steady phase of the r-process (figure 1b). It forms only after R falls below about 1, when steady β flow is destroyed and the path begins to move towards stability. The peak appears under a wide range of initial temperatures, densities, and neutron/seed ratios provided only that freezeout from

equilibrium is prompted by the capture of nearly all free neutrons rather than a sudden drop in overall density and temperature, as is often assumed. The primary reason is that, surprisingly, the r-process stays in approximate $(n, \gamma) - (\gamma, n)$ equilibrium even after steady flow fails. Only when R has fallen by many orders of magnitude does β decay completely dominate the other reactions and destroy the remnants of $(n, \gamma) - (\gamma, n)$ equilibrium. As a result, the path continues for some time to lie roughly along contours of constant neutron separation energy even as β decay moves it moves towards stability.

Figure 2 illustrates this phenomenon; it shows the path between $N = 82$ and 126 at three times during a 0.25-second interval just after the steady phase ends. During this period, as indicated by the insert in figure 2, R (or Y_n) drops dramatically (the diamonds mark the three times at which the path is plotted). The dark squares in the large figure are the paths as defined above, with the upper set corresponding to the later time. The open diamonds indicate the “equilibrium paths”, i.e. those that would obtain if the system were in true $(n, \gamma) - (\gamma, n)$ equilibrium according to Eq. (1). Contours of constant neutron separation energy for the even N nuclei are overlaid. The actual and equilibrium paths indeed differ very little well after the end of the steady phase. Eventually, as the figure shows, a “kink” in the separation energies at $N \approx 104$ is intercepted and imposes itself on the path.

Large kinks in the path are the underlying cause of the abundance peaks at the neutron closed shells mentioned above. Because the neutrons in all these nuclei are strongly bound the path turns sharply up towards stability when a closed shell is reached, producing a concentration of populated isotopes close together in A with relatively long β -decay lifetimes. The early explanation of the REE peak in Ref. [3] is a variation on the same theme. In our simulations, however, the REE peak does not form in exactly this way, even though it is clearly associated with the $N \approx 104$ kink, which in turn is clearly due [10] to the deformation maximum postulated in Ref. [3]. The nuclei at the top of the kink, and thus closer to stability, do have moderately slower β -decay rates than those along the path immediately below, but neither this fact nor the proximity of the kink nuclei to one another along the path account entirely for the pronounced REE peak. Another mechanism, connected with the motion of the path as it traverses the kink, is also at work.

In the vicinity of the kink the average separation energy that determines the equilibrium path grows at a rate governed by the beta decay of an “average-lifetime” nucleus, which is typically in the kink. Below the kink, as just mentioned and illustrated in the center of figure 3, the nuclei along the path are farther from stability and therefore decay faster than average, before the average separation energy has changed enough to move the equilibrium path in their vicinity. In an attempt to return to the path and stay in equilibrium, these nuclei then capture neutrons (which are rapidly dwindling in number), increasing their value of A . The nuclei above the kink, by contrast, decay more slowly than average, and in general will not do so before the equilibrium path at their location has moved. When it does move, these nuclei, whose thermodynamic impetus is also to remain in equilibrium at the average separation energy, photodisintegrate so that their mass number A is lowered. The net result, shown with arrows in the insert in figure 3, is a funneling of nuclei into the kink region as the path moves toward stability.

To confirm these ideas, we ran a simulation with our own simplified and easily varied nuclear properties. We obtained binding energies from a simple semi-empirical mass formula ([12]) and β -decay lifetimes by fitting those of Ref. [10] with a function of the form $T_{1/2} =$

aQ^α , where Q is the difference in binding energies between the parent and daughter and the best fit was obtained with $a = 250$ and $\alpha = -3.80$. We assumed neutron capture rates, the details of which are irrelevant, to have an exponential dependence on separation energy, reflecting their dependence on the level density in the compound nucleus formed by capture. We started the simulation at the end of the steady phase of the r-process, with abundances along the equilibrium path between $N = 82$ and $N = 126$ taken to be identically normalized Gaussians of width 1.05 centered at N_{max} for each Z . These conditions produced a flat final abundance curve, shown in figure 4a alongside the (appropriately scaled) solar abundances. When we introduced a kink into the separation energies at $N = 104$, adjusting the capture and β -decay rates to reflect the new bindings, a REE peak matching that in the solar-abundance curve formed (figure 4b). But when we modified the β -decay rates to be constant along curves of constant separation energy, destroying the β -decay-induced dynamic described above, the peak shrank by a factor of about 2 relative to the surrounding abundance level (figure 4c). This smaller peak therefore represents the effects of the concentration of points along the path and the slight increase in β -decay lifetimes at the top of the kink. These factors alone are clearly not enough to fully produce the peak.

The simplified set of freezeout-related calculations just described summarizes the necessary and sufficient conditions for the formation of a REE peak with the correct size. We conclude that this peak is indeed due to a deformation maximum in the region, but that in order for it to form the maximum must be traversed after the steady phase of the r-process ends but before the system completely freezes out of $(n, \gamma) - (\gamma, n)$ equilibrium.

Nuclear physics has often contributed to our understanding of the r-process, and vice versa. Through the study of certain β -decay rates, for example, the authors of Ref. [13] provided experimental support for the idea that the r-process distribution contains many components. On the other hand, observed r-process abundances near $A \approx 120$ apparently say something significant about the strength of the closed $N = 82$ shell near the neutron-drip line [14]. These important discoveries have all involved the steady phase of the r-process (but see Ref. [15]). By contrast the REE peak is associated with freezeout, and is therefore sensitive to conditions at later times. The work reported here allows us to conclude, for instance, that freezeout is prompted by the exhaustion of free neutrons rather than a rapid drop in overall density and/or temperature. This fact may constrain models in which the expansion of the r-process region is so fast that freezeout occurs before nearly all the neutrons have been captured. The existence of the peak also confirms the predicted deformation of neutron-rich rare-earth nuclei, and its fine structure may constrain nuclear models. Finally, the effect on the REE peak of neutrinos emitted from the cooling supernova remnant has yet to be examined. The delicate interplay of nuclear deformation, neutron capture, photodisintegration, and β decay that forms the REE peak as the r-process freezes out may thus have more to tell us about the conditions under which heavy-element nucleosynthesis occurs.

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FIGURES

FIG. 1. Calculated (line) and measured (crosses) solar r-process abundances. Part a) shows the final calculated abundances and part b) the calculated abundances before freezeout, while the r-process is in the steady phase.

FIG. 2. The r-process path between $N = 82$ and 126 at three times during a 0.25-second interval early in the decay to stability. The shaded squares are the actual paths, the lightest corresponding to the latest time, and the diamonds the equilibrium paths defined at the same times by Eq. (1). The lines are contours of constant separation energy in MeV. The insert shows the neutron abundance per nucleon over this interval, with the three times at which the path is depicted indicated by diamonds.

FIG. 3. Contours of constant neutron separation energy in MeV (solid lines) and constant β -decay rates in s^{-1} (dashed lines). The insert is a schematic of two such contours, with the arrows depicting the flow of nuclei into the region containing the separation-energy kink.

FIG. 4. Abundances on a linear scale near $A = 160$ in the simplified model (see text). Part a) is with smooth separation-energy contours, part b) with a kink in the contours, and part c) with constant β -decay rates along each kinked contour. The crosses are the appropriately scaled solar abundances.







